Thin Solid Films 612 (2016) 116–121

Contents lists available at ScienceDirect

Thin Solid Films

journal homepage: www.elsevier.com/locate/tsf

Analysis of X-ray diffraction curves of trapezoidal Si nanowires with a strain distribution

Teruaki Takeuchi [a,*], Kosuke Tatsumura [b,1], Takayoshi Shimura [c], Iwao Ohdomari [b,2]

[a] Research organization for Nano & Life innovation, Waseda University, 120-5, 513 Wasedatsurumaki-cho, Shinjuku-ku, Tokyo 162-0041, Japan
[b] Faculty of Science and Engineering, Waseda University, 3-4-1 Ohkubo, Shinjuku-ku, Tokyo 169-8555, Japan
[c] Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita-shi, Osaka 565-0871, Japan

ARTICLE INFO

Article history:
Received 3 July 2015
Received in revised form 27 May 2016
Accepted 27 May 2016
Available online 1 June 2016

Keywords:
X-ray diffraction
Silicon
Nanowires
Strain distribution
Trapezoidal cross-section

ABSTRACT

X-ray diffraction curves of oxidized Si nanowires with a strain distribution having a trapezoidal cross-section are analyzed using an X-ray kinematical treatment. The analysis is carried out assuming a strain distribution and cross-sectional shape to calculate a diffraction curve, followed by comparing it to the experimental one. The calculated diffraction curves reproduce the experimental ones over the whole measured range. Particularly, the calculated intensities as well as positions of fringe maxima and minima agree with the experimental curves. Also, the calculation indicates that the strain on a plane parallel to the bases becomes larger, as the plane becomes far from the longer base. This is demonstrated only by calculating X-ray diffraction curves assuming both strain distributions and cross-sectional shapes.

1. Introduction

In the field of Si micro devices, the strain engineering of Si crystal lattice is of both technological and scientific importance. The electronic band structure of Si can be modified by a small strain of Si. The mobility enhancement of electrons and holes caused by this effect is the crux of strained-Si MOSFET devices for high-performance ULSIs [1,2]. Also, the progress of oxidation in Si nano-structures strongly depends on the local stress [3,4]. Self-limiting oxidation is one of the most remarkable phenomena. By utilizing the self-limiting oxidation, a silicon single-electron transistor device operational at room temperature was fabricated [5,6].

To investigate the strain in Si nanostructures, X-ray diffraction is one of the most suitable techniques because sensitive and nondestructive measurements are possible [7,8]. In most X-ray diffraction experiments for nanowires [9–11], the obtained information reported on strain has been an average value. However, oxidized nanowires should have distributed strains, because the strain depends on the surrounding SiO_2 thickness which changes with position in a nanostructure [4]. Actually, a theoretical analysis indicates a distributed stress in a nanowire [12].

In order to determine strain distributions in nanowires, we have analyzed X-ray diffraction curves focusing on the intensity ratios of fringe maxima and the positions [13]. Such an analysis has provided good fittings to experimental fringe maxima, and strain distributions have been found to some extent. However, the intensities of minima have been ambiguous in the calculated diffraction curves. Also, it has been unknown whether the strain near the shorter base is larger than that near the longer base, although this has been determined practically, considering the growth process of surrounding SiO_2.

These problems appear to be solved by assuming the nanowire cross-sectional shapes [14–16] in addition to strain distributions. In the present work, both a strain distribution and cross-sectional shape are assumed simultaneously, and compare a calculated diffraction curve to the experimental one.

2. Experimental details

The nanowire samples were fabricated on a (001)-oriented silicon-on-insulator (SOI) wafer with a nominal 50 nm thick Si layer. Patterning was done by electron-beam lithography, followed by tetramethylammonium-hydroxide etching, employing a patterned thermal oxide layer as a mask. The samples were oxidized at 850 °C for an oxidization time of 1 and 5 h. These samples have Si nanowires along the [110] direction, as shown in Fig. 1(a), at a periodicity of 300 nm in the area of 15 × 15 mm^2. The nanowire cross-sectional shape is close to a trapezoid and the bases are parallel to the Si substrate.

* Corresponding author.
E-mail address: t-takeuchi@waseda.jp (T. Takeuchi).
[1] Present address: Advanced LSI Technology Laboratory, Corporate Research and Development Center, Toshiba Corporation, 1 Komukai-Toshiba-cho, Saiwai-ku, Kawasaki 212-8582, Japan.
[2] Present position: Professor emeritus at Waseda University.

http://dx.doi.org/10.1016/j.tsf.2016.05.047
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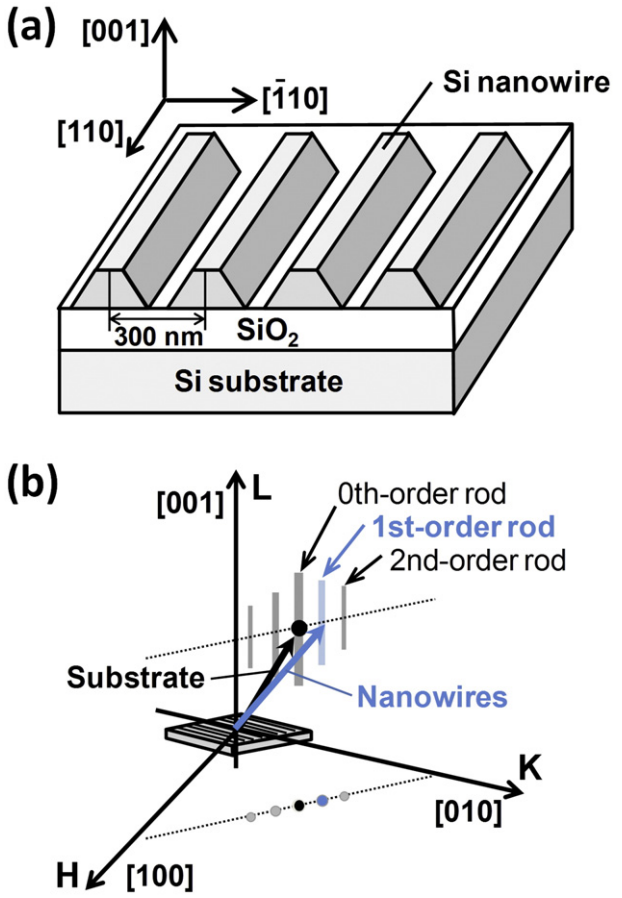

Fig. 1. (a) Schematic illustration of Si nanowires arranged at a periodicity of 300 nm in the [$\bar{1}$10] direction on a (001)-oriented SOI wafer. The nanowire cross-section is close to a trapezoid with bases parallel to the Si substrate. (b) Rod-shaped diffractions caused by nanowire periodicity around the 111 Bragg point. The diffraction of the first-order rod is separated from the Bragg reflection of the underlying Si substrate in reciprocal space.

The X-ray diffraction experiments are similar to those reported in Refs. [10,13]. The diffraction intensity around the 111 Bragg point for an X-ray with a 0.154 nm wavelength was measured using synchrotron radiation on the beam line BL4C at Photon Factory in the National Laboratory for High Energy Physics (KEK). A periodic arrangement gives rise to higher-order diffractions in addition to the ordinary 111 Bragg diffraction. These higher-order diffractions are elongated in the L direction, i.e. the [001] direction due to small thickness of the Si layer, as shown in Fig. 1(b). These rod-shaped diffractions are aligned in the direction based on the nanowire arrangement, as shown in the figure. By observing one of them, a mixture of the strong diffraction from the Si substrate is avoided.

If there is the periodic strain in the Si substrate by the nanowire formation, it is difficult to separate the signal of its satellites from that of the satellites produced by the periodic strain in oxidized nanowires. However, the experiments for unoxidized nanowire samples indicated that the diffraction curves of the first-order rod in nanowires were the same as the predicted ones [16]. Therefore, the consideration of the periodic strain produced in the Si substrate is not necessary. This is because there is an SiO_2 layer as thick as 135 nm between the nanowires and the Si substrate in the SOI wafer.

Preliminary experiments indicate that the separation of the first-order diffraction from the diffraction of the Si substrate is sufficient. Therefore, we have measured the first-order diffraction intensities, considering the fact that the diffraction intensity is larger in a lower-order diffraction.

The measurement of the first-order diffraction intensity was done as follows. One measurement point of the diffraction curve along the first-order rod consisted of 100-point measurements along a line across this rod, and we made the integrated value the intensity at this point. The whole diffraction curve which was plotted as the relation between the integrated value and L consisted of 80 points, and the measurement time was approximately 40 min.

3. Calculation

We assume that the [$\bar{1}$10] and [111] directions on the ($\bar{1}\bar{1}$2) plane are parallel to U and V coordinates respectively, as shown in Fig. 2. And we write the U component of the momentum transfer $\boldsymbol{q}$ as q_u and the V component as q_v. In a kinematical treatment, the diffraction intensity as a function of momentum transfers q_u and q_v is expressed as [17]:

$$I(q_u, q_v) = |f(q_u, q_v)|^2 \left| \frac{\sin(Nq_uP/2)}{\sin(q_uP/2)} \right|^2, \quad (1)$$

where $f(q_u, q_v)$ is the scattering amplitude from a single nanowire and the fraction including sinusoidal functions expresses the interference of diffracted X-rays from nanowires, which corresponds to the higher-order diffractions appearing at intervals of $2\pi/P$ in reciprocal space. This fraction is a constant if the number of order is given. P is the nanowire arrangement period and N is the number of nanowires in the coherence length of the X-ray beam.

Numerical calculations have been made based on the following assumptions. The (111) lattice spacing, namely, the distance between an atomic plane parallel to the trapezoidal bases and that adjacent to this atomic plane is the same, even if the in-plane position is different, as shown in Fig. 2. Under this condition, $f(q_u,q_v)$ is proportional to

$$A(q_u, q_v) = F_{111} \sum_{n=0}^{n_h} \left[\exp(2\pi i q_v v_n) \bullet \sum_{m=m_0}^{m_1} \exp(2\pi i q_u u_m) \right], \quad (2)$$

where, F_{111} is the crystal structure factor for the reciprocal lattice vector 111 and v_n is the distance between nth plane and the longer base of the trapezoid. The parameter m stands for the vertical lattice plane, and m_0 and m_1 correspond to the left and right ends of the colored thin rectangle, whose u-coordinates are u_0 and u_1, as shown in the figure. In the double summation, the summation with respect to m is n-dependent because m_0 and m_1 change with changing v. The strain in the [111] direction is expressed as $(v_{n+1} - v_n)/d_{111}$, where d_{111} is the (111)-interplanar distance of perfect crystal.

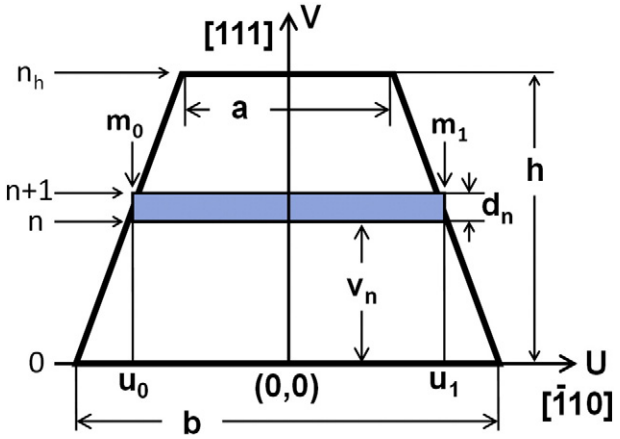

Fig. 2. Schematic illustration of the trapezoidal nanowire ($\bar{1}\bar{1}$2) plane on which the summation is performed. The (111) lattice spacing d_n is the same throughout the colored thin rectangle.